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Superelastic electron scattering from potassium atoms

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Abstract : We have carried out distorted wave (DW) calculations for the electron impact 4 ^2S–4 ^2P resonance excitation of potassium. The results for alignment and orientation parameters are obtained and compared with the very recent superelastic electron scattering measurements from the laser excited 4 ^2P states of potassium. The validity of DW method is commented upon.

Keywords . Electrons, excitation, Stokes parameters, alignment and orientation

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1. Introduction

There has been number of theoretical investigations to study resonance excitation in potassium by impact of electrons [1–3] These have included distorted wave methods and close coupling calculations. Due to limited availability of experimental data the methods seem to work successfully only in certain energy range as demonstrated by Stockman *et al* [4] through the comparison of their measurements on potassium for Stokes parameters at the electron energies of 10 and 54.4 eV.

Very recently Stockman *et al* [5] have therefore extended their experimental study in the wide energy range up to 100 eV for certain electron scattering angles in order to provide testing of the suitability of different theoretical approximations for the resonance excitation in potassium. They measured angular dependence of the Stokes parameters and alignment and orientation parameters for the 4 ^2P state in potassium using superelastic technique. In their experiment a collimated beam of potassium atoms intersects a beam of electrons in the scattering plane, which is defined by the incident and scattered electron momentum directions. The vertically directed laser beam of wavelength 766.701 nm crosses the atom and electron beams normal to the scattering plane. The laser radiation excites the potassium atoms from the ground 4 ^2S state to the 4 $^2P_{3/2}$ state having excitation energy equal to 1.6 eV. Those electrons that gain 1.6 eV in energy, the superelastic electrons, in the collision with the excited atoms, are detected at selected scattering angles for six different laser polarization states. The intensity of superelastic electrons detected at each scattering angle and the polarization of the decay fluorescence analyzed in the scattering plane is used to determine the reduced Stokes parameters [6,7]. Thus such measurements provide a complete set of the four spin averaged parameters which fully characterize the electron impact excitation of the 4 ^2S–4 ^2P transition.

In the light of the experiment of Stockman *et al* [5] we have carried out distorted wave approximation calculations for electron impact excitation of the 4 ^2S–4 ^2P transition in potassium and present comparison of our results with the experiment for the reduced Stokes parameters and alignment and orientation parameters. In order to be brief, here, we outline the theoretical considerations and report our selected results only. The extensive presentation with full details will be given in our later publication.

2. Theoretical considerations

2.1. *Distorted wave theory :*

We treat the potassium atom as one electron system and consider the electron impact 4 ^2S–4 ^2P excitation as due to

excitation of the valence $4s$ electron to the $4p$ orbital. In this process effect of core electron is taken through the core potential. Transition matrices for electron impact excitation of potassium from initial state (i) to a final state (f), for the singlet (s) and triplet (t) modes can be written as

$$T^{s}_{ifM} = T^{d}_{ifM} + T^{ex}_{ifM} \quad \text{(singlet mode)} \tag{1}$$

$$T^{t}_{ifM} = T^{d}_{ifM} - T^{ex}_{ifM} \quad \text{(triplet mode)} \tag{2}$$

where T^{d}_{ifM} and T^{ex}_{ifM} are the spin averaged direct and exchange matrices in distorted wave approximation. $M = 0, \pm 1$ refers to the magnetic components of the excited $4\ ^2P$ state. These can be further written as

$$T^{d}_{ifM} = \left\langle F^{-}(\boldsymbol{k}_f, \boldsymbol{r}_2)\phi_{fm}(\boldsymbol{r}_1)\middle| V - U_f(\boldsymbol{r}_2)\right| \times \phi_i(\boldsymbol{r}_1)F^{+}(\boldsymbol{k}_i, \boldsymbol{r}_2)\Big\rangle \tag{3}$$

and

$$T^{ex}_{ifM} = \left\langle F^{-}(\boldsymbol{k}_f, \boldsymbol{r}_2)\phi_{fm}(\boldsymbol{r}_1)\middle| V - U_f(\boldsymbol{r}_2)\right| \times \phi_i(\boldsymbol{r}_2)F^{+}(\boldsymbol{k}_i, \boldsymbol{r}_2)\Big\rangle \tag{4}$$

where V is the total interaction potential between the target potassium atom and the projectile electron and can be expressed as

$$V = -\frac{1}{r_2} + \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} + V^{\text{core}}(r_2) \tag{5}$$

where $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are respectively the position co-ordinates of the target and projectile electrons with respect to the target nucleus. The core potential V^{core} of the potassium atom is taken as defined in reference [1].

$F^{\pm}_{i(f)}(\boldsymbol{k}_{i(f)}, \boldsymbol{r})$ is the initial (final) channel projectile electron distorted wave with the wave vector $\boldsymbol{k}_{i(f)}$ and satisfies the following differential equation

$$\left[\nabla^2 + k^2_{i(f)} - 2U_{i(f)}\right]F^{\pm}(\boldsymbol{k}_{i(f)}, \boldsymbol{r}) = 0 \tag{6}$$

Here $U_{i(f)}$ is the distortion potential for the initial (final) channel and chosen as

$$U_{i(f)} = V^{\text{stat}}_{i(f)} + V^{\text{exch}}_{i(f)} \tag{7}$$

where $V^{\text{stat}}_{i(f)}$ is the static potential in the initial (final) channel and is obtained from the initial (final) state of the potassium atom

$$V_{i(f)} = \left\langle \phi_{i(f)}|V|\phi_{i(f)}\right\rangle \tag{8}$$

The following expression for exchange potential $V^{\text{exch}}_{i(f)}$ in the initial (final) channel is taken [8]

$$V^{\text{exch}}_{i(f)} = \frac{1}{2}\left\{\left(\frac{1}{2}k^2_{i(f)} - V^{\text{stat}}_{i(f)}\right) - \left[\left(\frac{1}{2}k^2_{i(f)} - V^{\text{stat}}_{i(f)}\right)^2 - 8\pi\tau\rho_{i(f)}\right]^{1/2}\right\} \tag{9}$$

$\rho_{i(f)}$ is spherically averaged charged density of the potassi atom in the initial (final) channel and τ is taken +1 and respectively for singlet and triplet modes [9].

The scattering amplitude a_M is related to the t transition matrix through the following relation

$$a^{s(t)}_{M} = -\left(\frac{1}{2\pi}\right)T^{s(t)}_{ifM}$$

Finally, the spin-averaged amplitude $\langle a_{M'}, a^{*}_{M}\rangle$ is gi by

$$\langle a_{M'}, a^{*}_{M}\rangle = \frac{1}{2(2S_i+1)}\sum(2S+1)a^{s}_{M'}a^{s*}_{M}$$

where S_i is the atomic spin in the initial state and S is total spin of the system *i.e.* $S = 0$ for singlet mode $S = 1$ for triplet mode.

2.2. *Stokes parameters and alignment and orienta parameters :*

Further, the polarization of the light emitted from decay of the excited $4\ ^2P$ state in a particular direc can be completely described by the following Sto parameters

$$P_1 = \frac{I(0°) - I(90°)}{I(0°) + I(90°)}$$

$$P_2 = \frac{I(45°) - I(135°)}{I(0°) + I(135°)}$$

$$P_3 = \frac{I(\text{RHC}) - I(\text{LHC})}{I(\text{RHC}) + I(\text{LHC})}$$

where $I(\phi)$ is the intensity of light with polarizat vector in the ϕ direction with respect to incident elec direction and I(RHC) and I(LHC) are respectively intensities of the right and left circularly polarized l components.

These Stokes parameter P_1–P_3 can be related to excitation amplitudes through the following relation, say the decay $L \rightarrow L_2$

$$= \frac{1}{I^{Y}}\begin{Bmatrix} 1 & 1 & 2 \\ L & L & L_2 \end{Bmatrix} : \left[\sqrt{\frac{3}{2}}G_2(L)\left\langle T(L)^{+}_{20}\right\rangle - G_2(L)\left\langle T(L)^{+}_{22}\right\rangle\right]$$

$$P_2 = \frac{1}{I^{Y}}\begin{Bmatrix} 1 & 1 & 2 \\ L & L & L_2 \end{Bmatrix}\left[2G_2(L)\left\langle T(L)^{+}_{21}\right\rangle\right]$$

$$P_3 = \frac{1}{I^{Y}}\begin{Bmatrix} 1 & 1 & 1 \\ L & L & L_2 \end{Bmatrix}\left[2iG_1(L)\left\langle T(L)^{+}_{11}\right\rangle\right]$$

$$\text{where } I^{\gamma} = \frac{2(-1)^{L+L_2}}{3(2L+1)^{1/2}} G_0(L)\left\langle T(L)^{\dagger}_{00}\right\rangle + \begin{Bmatrix} 1 & 1 & 2 \\ L & L & L_2 \end{Bmatrix} \times \left[\frac{G_2(L)}{\sqrt{6}}\left\langle T(L)^{\dagger}_{20}\right\rangle + G_2(L)\langle T(L)\rangle\right] \quad (18)$$

The depolarization coefficient $G_K(L)$ can be written as

$$G_K(L) = \frac{1}{(2S+1)}\sum_J (2J+1)^2 \begin{Bmatrix} L & J & S \\ J & L & K \end{Bmatrix} \quad (19)$$

S is the electronic spin and $J = L + S$ is the total angular of the atom. The $G_K(L)$ are normalized such that $G_0(L) = 1$ for all value of L. $\left\langle T(L)^{\dagger}_{KQ}\right\rangle$ is the state multipoles of the excited state with angular momentum L are related to the complex scattering amplitude as

$$\left\langle T(L)^{\dagger}_{KQ}\right\rangle = \sum_{M',M}(-1)^{L-M'}(2K+1)^{1/2} \times \begin{Bmatrix} L & L & K \\ M' & -M & -Q \end{Bmatrix}\left\langle a_{M'}, a^{*}_{M}\right\rangle \quad (20)$$

To describe the alignment and orientation of the charge cloud of the excitation 4 ^2P state of potassium, we use the Andersen parameters [10] which are related to the Stokes parameters by the following relations

$$\gamma = \frac{1}{2}\arg\left(\bar{P}_1 + i\bar{P}_2\right) \quad (21)$$

$$P_l = \left(\bar{P}_1^2 + \bar{P}_2^2\right)^{1/2} \quad (22)$$

$$L_{\perp} = -\bar{P}_3 \quad (23)$$

$$P^{+} = \sqrt{\bar{P}_1^2 + \bar{P}_2^2 + \bar{P}_3^2} \quad (24)$$

$\bar{P}_1 - \bar{P}_3$ are the reduced Stokes parameters which may be obtained by using the same relations (eqs.15–17) as for measured Stokes parameters $P_1 - P_3$ but with all $G_K(L)$taken as unity.

Results and discussion

Stockman *et al* [5] measured the reduced Stokes parameters for electron scattering angles of 45, 60 and 90 degrees, respectively. The energy of the incident electrons was up to 84 eV, which corresponds to 100 eV for the superelasticaly scattered electrons. In Figure 1, we compare their experimental data for reduced Stokes parameters at 45 degree of scattering with our distorted wave calculations. In order to see the effect of electron exchange effect in the distortion potential we present our two types of calculations *i.e.* with exchange potential (DWE) and without (DW). From the figure, we find that for $\bar{P}_1$ parameter, the DWE results are in the perfect over all agreement with the experiment. For $\bar{P}_2$ parameters, our both the calculations are in satisfactory agreement for energies above 30 eV of energy, although the nature observed for the experimental data is reproduced. Finally, for $\bar{P}_3$ parameter, both the calculations are in good

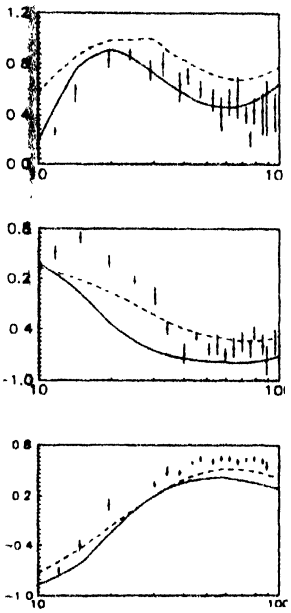

Figure 1. The reduced Stokes parameters $\bar{P}_1$, $\bar{P}_2$ and $\bar{P}_3$ for electron impact 4 ^2S–4 ^2P excitation in potassium at a fixed scattering angle of 45 degree. The electron energy refers to the energy of the superelastic electrons. Solid circles are experimental data from Stockman *et al* [5]. The dashed and solid lines respectively are our DWE and DW calculations.

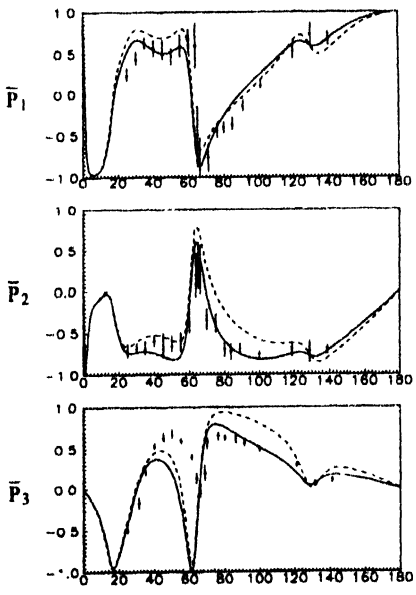

Figure 2. The reduced Stokes parameters $\bar{P}_1$, $\bar{P}_2$ and $\bar{P}_3$ for electron impact 4 ^2S–4 ^2P excitation in potassium for superelastic electron energy of 80 eV. The captions are as in Figure 1.

agreement with experiment. We also observe as expected that the DWE calculations can be said to be better than the DW. Results at other scattering angles are not compared and discussed in this paper.

As an additional study Stockman *et al* [5] also measured the angular dependence of the Stokes parameters at an incident electron energy of 78.4 eV *i.e.* superelastic electron energy of 80 eV. We compare in Figures 2 and 3, their experimental results for reduced Stokes parameters $\bar{P}_1$, $\bar{P}_2$, $\bar{P}_3$ and alignment and orientation parameters (*viz.* γ, P_ℓ and P^+ only, as $L_\perp = -\bar{P}_3$) with our distorted wave calculations. We find that our DWE calculations reproduce the experimental results excellently. Being high energy the DWB and DW calculations are also very close.

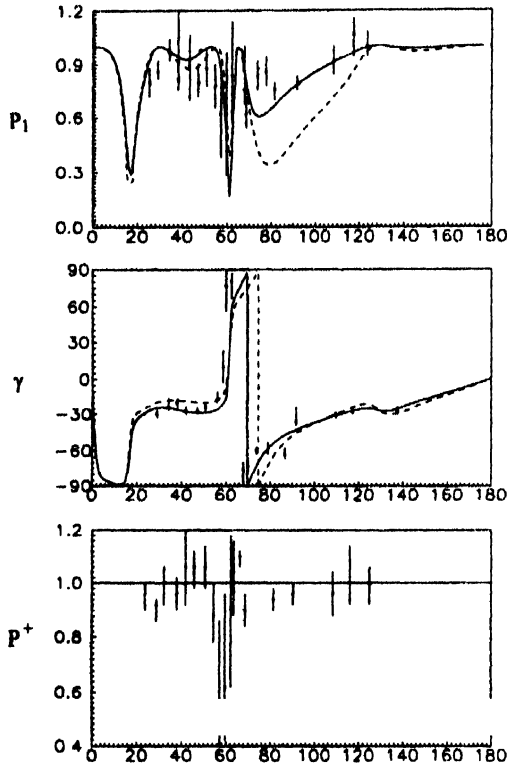

Figure 3. The P_ℓ, γ (degrees) and P^+ parameters for the electron impact excited 4 ^2P state of potassium for superelastic electron energy of 80 eV. The captions are as in Figure 1.

4. Conclusion

The present study suggests that DW theory can describe the 4 ^2S–4 ^2P excitation in potassium atom for a wide range of incident electron energies as it satisfactorily reproduces the recent experimental results.

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